Nuclear Reaction Model Code EMPIRE-II

(version: 2.19beta10 Lodi)

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EMPIRE developers

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EMPIRE highlights

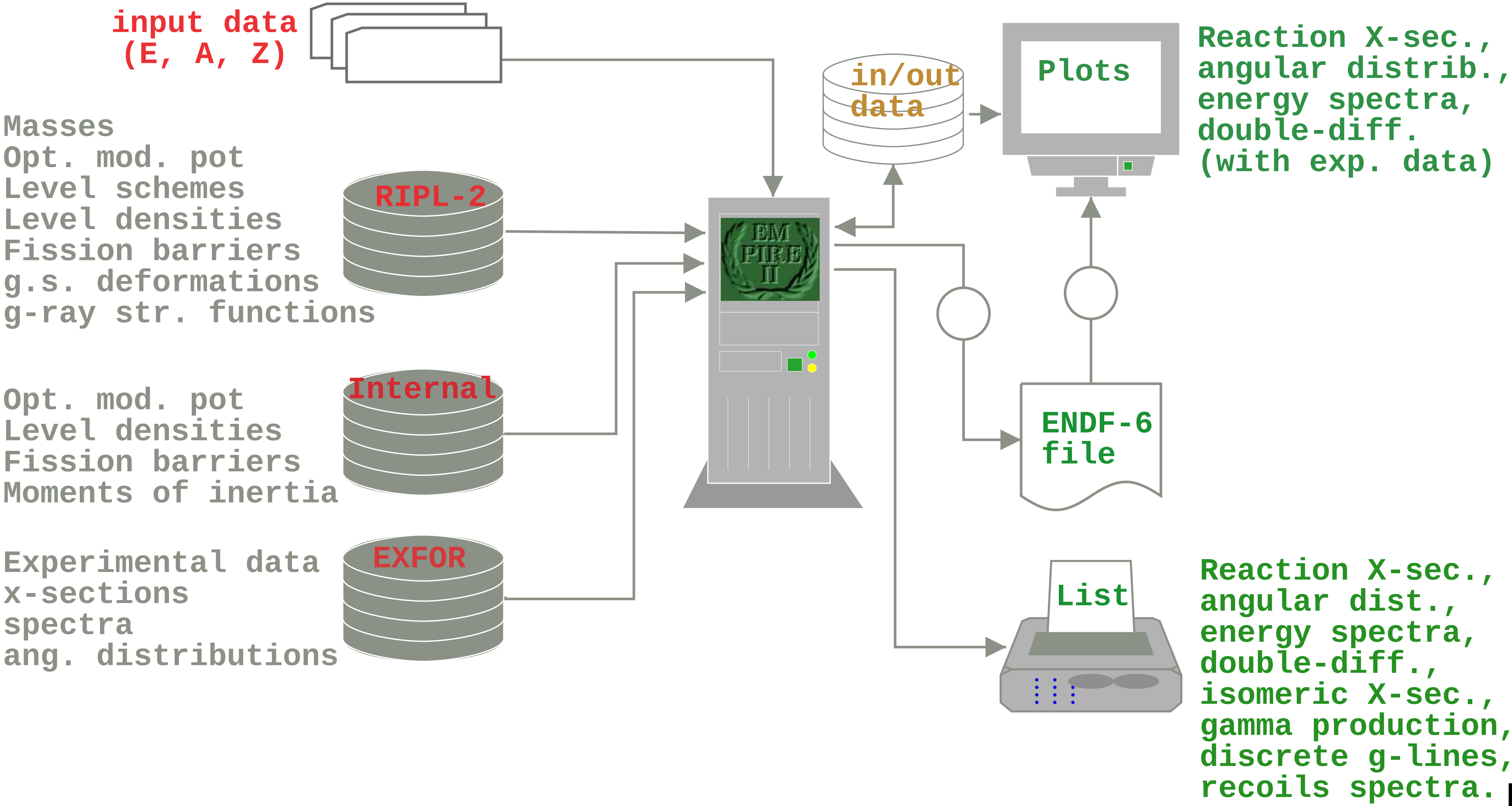
System of codes for modeling nuclear reactions:

- broad range of energies (up to ~200 MeV) and projectiles (any nucleon or HI)
- most important nuclear reaction models
- extensive input parameter library (RIPL-2)
- ENDF-6 formatting
- utility codes (ENDF-6 verification)

EMPIRE highlights (cont.)

- automatic retrieval of experimental data from EXFOR
- interactive plots of experimental and calculated results
  - excitation functions
  - angular distributions
  - inclusive emission spectra for n, p, α, and γ)
  - double differential spectra

EMPIRE layout



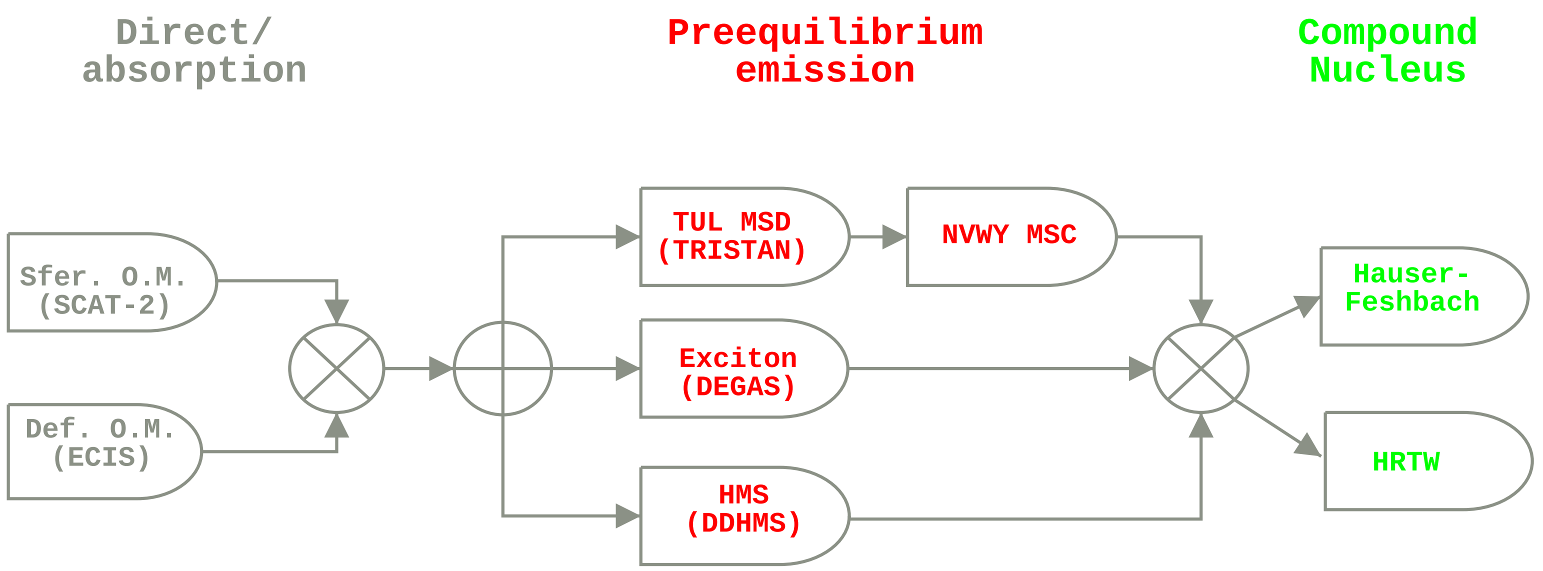
Reaction mechanisms

- optical model (SCAT2),
- coupled channels (ECIS),
- TUL Multistep Direct (ORION + TRISTAN),
- NVWY Multistep Compound with γ-emission,
- second-chance preeq. emission,
- exciton model (DEGAS),

Reaction mechanisms (cont.)

- Monte Carlo preequilibrium (DDHMS),
- HRTW for widths' fluctuations,
- Hauser-Feshbach model with full γ-cascade and dynamical deformation effects ,
- State of the art fission (three-hump barrier)

EMPIRE core

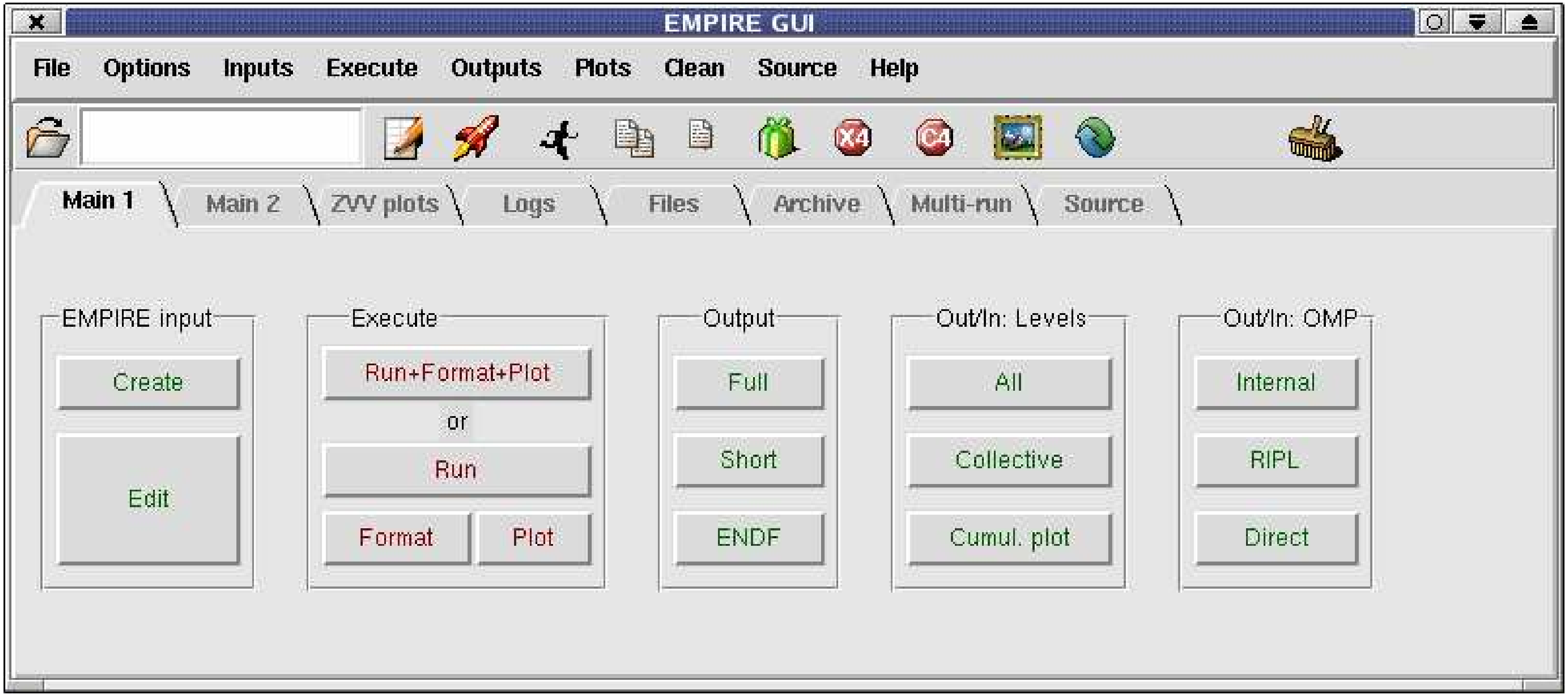


CC MSD MSC DEGAS HMS Lev.Den.

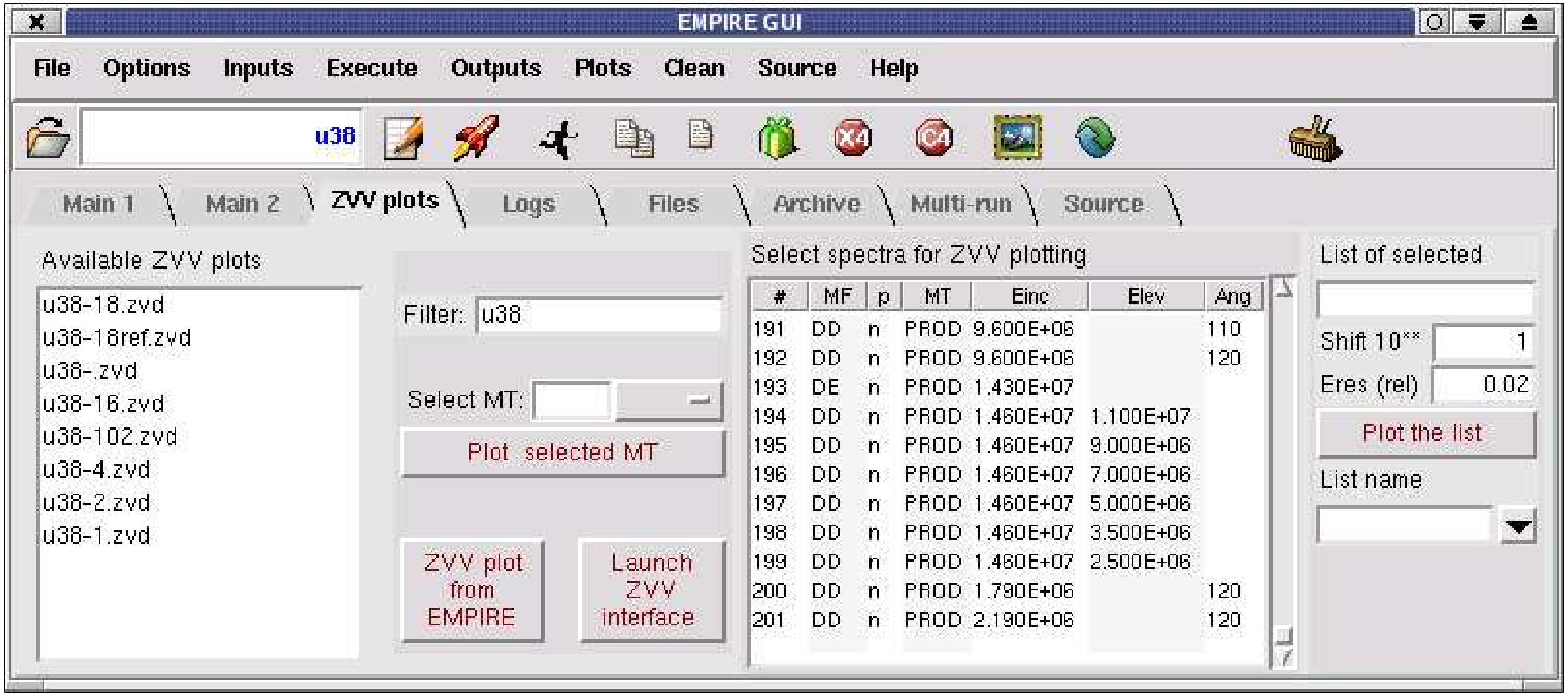
EMPIRE statistics

- EMPIRE core: >60 000 lines
- utility codes: >61 000 lines
- # of bash and Tcl/Tk scripts: 25
- size of the internal parameter library: 2 Mb
- size of the RIPL-2 library: 224 Mb
- size of the EXFOR library: 567 Mb

EMPIRE GUI (Main)



EMPIRE GUI (ZVV plots)



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Operating systems

- languages: FORTRAN 77 (99%), C (mostly ZVView), bash, Tcl/Tk, awk
- operating systems:
  - **Linux** (developed on Red Hats up to version 9),
  - UNIX (any one should work but TLC might be needed)
  - Mac (reported to work)
  - MS Windows (EMPIRE core runs)
  - VMS (EMPIRE core used to run)

Coupled-Channels and DWBA

ECIS code by J. Raynal

- Important for deformed nuclei
- Provides:
  - total cross section
  - elastic cross section
  - absorption cross section
  - inelastic cross sections to collective levels
  - transmission coefficients

CC and DWBA (cont.)

- EMPIRE calls ECIS in a transparent way
- RIPL or internal omp are used
- Collective levels taken from RIPL or set up automatically
- Deformed nuclei treated as rotational, spherical as vibrational
- Results are transferred to EMPIRE and used in subsequent calculations

CC and DWBA (cont.)

ECIS can be invoked by EMPIRE in 3 ways:

DIRECT=1 CC for collective levels, total, elastic and absorption, SCAT2 T_l's used for PE and HF calculations

DIRECT=2 as above but CC is used for all T_l's

DIRECT=3 DWBA for collective levels, total, elastic and absorption, SCAT2 T_l's used for PE and HF calculations.

Multistep Direct

ORION & TRISTAN by Tamura, Udagawa and Lenske (TUL)
Combination of:

- direct reaction (DR),
- microscopic nuclear structure
- statistical methods.

$\Downarrow$

MSD Highlights

$$H = H^{opt} + H^{intr} + V^{res} \quad .$$

- H^{opt} optical model part
- H^{intr} intrinsic Hamiltonian
- V^{res} residual effective projectile-target interaction

MSD Highlights (cont.)

Lippmann-Schwinger equation for the T-matrix

$$T^{(n)}_{\gamma 0} = < \chi^{(-)}_E |(\gamma| V^{res} (G^{chan}(E) V^{res})^{n-1} |0)| \chi^{(+)}_0 >$$

the $n-$step transition from the entrance channel with incoming wave $\chi^{(+)}_0$ and the ground state configuration $|0) = |aA)$ to an exit channel γ with outgoing wave $\chi^{(-)}_E$ at the energy E

- $G^{chan}(E)$ Green's function for the channel.
- Scattering waves are optical model wave functions.

MSD Highlights (cont.)

- Real states γ are expanded into *n*-particle *n*-hole model states *c*. With

$$H^{intr} = H_0^{intr} + V^{intr} \quad .$$

  model states c are eigenstates of H_0^{intr}

- Residual interaction V^{intr} couples states from different particle-hole classes only.
- Configuration mixing between $np - nh$ classes is of stochastic nature
- Never-come-back hypotheses

MSD Highlights (cont.)

- The one-step cross section is expressed as

$$\frac{d^2\sigma^{(1)}}{dE d\Omega} = \sum_{\lambda} S_\lambda(E) \overline{\frac{d\sigma^{(1)}}{d\Omega}} |_\lambda \,,$$

where $\overline{\sigma^{(1)}}$ is a reduced DWBA cross section calculated with the average form factors.

MSD Highlights (cont.)

- The final result for the two-step MSD cross section is of very intuitive structure

$$\frac{d^2\sigma^{(2)}}{dE d\Omega} = \sum_{\lambda_1 \lambda_2} \int dE_1 S_{\lambda_2}(E, E_1) S_{\lambda_1}(E_1, 0) \overline{\frac{d\sigma^{(2)}}{d\Omega}}(E, E_1) \mid_{\lambda_1 \lambda_2}.$$

$\overline{\sigma^{(2)}}$ is an averaged cross section defined in terms of the $T^{(2)}-$matrix elements

Response Functions

- A reliable description of response functions is provided by the Random Phase Approximation theory (RPA).
- RPA accounts for collective and non-collective features on the same theoretical footing (weakly excited background states and the strongly excited giant resonances (GR), low-lying surface vibrations).
- Energy weighted sum rules are conserved
- The enhancement of the response due to ground state correlations is included.

Response Functions (cont.)

- The quasi-particle RPA (QRPA) $\Rightarrow$ canonical transformation to two quasi-particle ($2qp$) rather than $1p - 1h$ states.
- $2qp$ energies are taken to be complex by adding a state dependent damping width $\Gamma_{\alpha}^{\downarrow}$.
- The MSD response functions are calculated with single particle levels from a spherical Nilsson Hamiltonian with standard parameters.
- Only inelastic events are considered.

MSD Implementation

- Input parameters are passed to ORION and TRISTAN directly from the EMPIRE.
- Default MSD calculation can be performed without any additional input.
- κ_0 self-consistent coupling
- κ_1 from GDR energy
- κ_2, κ_3, κ_4 from excitation energies of low-lying 2^+, 3^-, and 4^+collective levels.
- Charge exchange channels not allowed.

Multistep Compound

Nishioka, Verbaarschot, Weidenmueller, Yoshida (NVWY)

- series of transitions along the chain of classes of closed channels of increasing complexity.
- classes defined in terms of the number of excited particle-hole pairs (n) plus the incoming nucleon.

$$N = 2n + 1$$

- two-body force $\Rightarrow$ only neighboring classes are coupled $(\Delta n = \pm 1)$.

MSC (cont.)

- Average MSC cross-section

$$\frac{d\sigma_{ab}}{dE} = (1 + \delta_{ab}) \sum_{n,m} T_n^a \Pi_{n,m} T_m^b \,,$$

(kinematical and angular-momentum dependent factors omitted).

$\Downarrow$

MSC (cont.)

- The transmission coefficients T_n^a coupling channel a and class n are given as

$$T_n^a = \frac{4\pi^2 U_n^a}{(1 + \pi^2 \sum_m U_m^a)^2},$$

where
$U_n^a = \rho_n^b < W_{n,a} >$
ρ_n^b bound level density of class n,
$W_{n,a}$ the average matrix elements connecting channel a with the states in class n.

MSC (cont.)

- The probability transport matrix Π_{mn} is defined via its inverse,

$$\begin{aligned}(\Pi^{-1})_{nm} &= \delta_{nm}(2\pi\rho_n^b)(\Gamma_n^{\downarrow} + \Gamma_n^{ext}) \\ &\quad -(1-\delta_{nm})2\pi\rho_n^b \overline{V_{n,m}^2} 2\pi\rho_m^b \,.\end{aligned}$$

$\overline{V_{n,m}^2}$ matrix element coupling states in classes n and m,
$\Gamma_n^{\downarrow}$ average spreading width of states in n,
Γ_n^{ext} average total decay width in class n.

MSC (cont.)

- The spreading width $\Gamma_n^{\downarrow}$ is again related to the mean squared matrix element $\overline{V_{n,m}^2}$

$$\Gamma_n^{\downarrow} = 2\pi \sum_m \overline{V_{n,m}^2} \rho_m^b \,.$$

- Chaining hypothesis $\Rightarrow$ $\overline{V_{n,m}^2}$ couples only neighboring classes ($\overline{V_{n,m}^2} = 0$unless $\mid n - m \mid = 1$).

MSC (cont.)

- The decay width Γ_n^{ext} is determined by the sum of the transmission coefficients T_n^a over all open channels

$$\Gamma_n^{ext} = (2\pi\rho_n^b)^{-1} \sum_a T_n^a \,.$$

- Chaining hypothesis $\Rightarrow$ only $\mid n - m \mid \leq 1$ emissions are allowed.
- Note that, differently from the FKK formulation, in the NVWY theory transmission coefficients $T_{n\to m}$ carry two class indexes.

MSC (cont.)

- All microscopic quantities $< W_{n,a} >$ and $\overline{V_{n,m}^2}$ are expressed in terms of the macroscopic ones.
  - $< W_{n,a} >$ is equated to optical model transmission coefficient
  - $\overline{V_{n,m}^2}$ is related to the imaginary part of the optical model potential $W(\epsilon)$ with $\Gamma_n^{\downarrow} = 2W(\epsilon)$.

MSC (cont.)

- Matrix Π^{-1} is inverted numerically and used to calculate MSC emission spectra.
- EMPIRE decides whether the MSC should be followed by the Hauser-Feshbach or not.

CC MSD MSC DEGAS HMS Lev.Den. Results

Exciton Model

- DEGAS code by E.Betak and P. Oblozinsky
- Semi-classical PE model for nucleon induced reactions
- Strict angular momentum coupling (FKK-like)
- EMPIRE version limited to:
  - single PE emission
  - primary γ-cascade
  - 4 exciton stages

Exciton Model (cont.)

- Absorption cross section renormalized to the EMPIRE one
- Results:
  - neutron, proton and γ spectra
  - spin dependent population of residuals
- Proved to give γ-spectra similar to more microscopic Direct-Semidirect model
- Applicable up to about 30 MeV

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Monte Carlo Preequilibrium

- Formulated by M. Blann and coded by M. Chadwick
- Unlimited multiple precompound emissions
- Residuals' production for nucleon induced reactions
- Double-differential spectra
- Recoil spectra
- Thermodynamically correct binding energies
- Applicable up to about 250 MeV

Dynamical approach to lev. dens.

(specific to EMPIRE)

- Features:
  - Collective enhancements due to nuclear vibration and rotation.
  - Super-fluid model below critical excitation energy
  - Fermi gas model above critical excitation energy
  - Rotation induced deformation (spin dependent)

Dynamical lev. dens. (cont.)

- Prolate nuclei

$$\rho(E,J,\pi) = \frac{1}{16\sqrt{6\pi}}\left(\frac{\hbar^2}{\Im_{||}}\right)^{\frac{1}{2}} a^{1/4} \sum_{K=-J}^{J}\left(U-\frac{\hbar^2K^2}{2\Im_{eff}}\right)^{-\frac{5}{4}}$$

$$\exp\left\{2\left[a\left(U-\frac{\hbar^2K^2}{2\Im_{eff}}\right)\right]^{\frac{1}{2}}\right\}.$$

Dynamical lev. dens. (cont.)

- Oblate nuclei

$$
\begin{aligned}
\rho(E,J,\pi) \; &= \; \frac{1}{16\sqrt{6\pi}}\left(\frac{\hbar^2}{\Im_{\|}}\right)^{\frac{1}{2}} a^{1/4} \\
& \sum_{K=-J}^{J}\left(U-\frac{\hbar^2\left[J\left(J+1\right)-K^2\right]}{2|\Im_{eff}|}\right)^{-\frac{5}{4}} \\
& \exp\left\{2\left[a\left(U-\frac{\hbar^2\left[J\left(J+1\right)-K^2\right]}{2|\Im_{eff}|}\right)\right]^{\frac{1}{2}}\right\}.
\end{aligned}
$$

Dynamical lev. dens. (cont.)

K - spin projection,
$\Im_{eff}$ - effective moment of inertia
defined in terms of perpendicular $\Im_{\|}$ and parallel $\Im_{\perp}$ moments

$$\frac{1}{\Im_{eff}} = \frac{1}{\Im_{\|}} - \frac{1}{\Im_{\perp}}.$$

Dynamical lev. dens.(cont.)

- Rotational enhancement automatically taken into account.
- Vibrational enhancement

$$K_{vib} = exp\left\{1.7\left(\frac{3m_0A}{4\pi h^2 S_{drop}}\right)^{2/3} T^{4/3}\right\}$$

with $S_{drop} = 17/4\pi r_{2_0}$ and $r_0 = 1.26$.

- Rotational and vibrational enhancements are damped with increasing energy

Super-fluid (BCS) lev. dens.

- Used below critical energy
- Level densities are expressed through the determinant Det calculated within the BCS theory

$$\rho_{BCS}(U,J) = \frac{2J+1}{2\sqrt{2\pi}\sigma_{eff}^3\sqrt{Det}} \exp\left(\frac{S - J(J+1)}{2\sigma_{eff}^2}\right)$$

- Corrected for rotational and vibrational collective effects in the non-adiabatic mode

$$\rho(U,J) = \rho_{BCS}(U,J) Q_{rot}^{BCS} K_{rot} Q_{vib} K_{vib} .$$

Level densities in EMPIRE

EMPIRE-specific:

- a energy dependent following Ignatyuk et al.
- a deformation dependent (surface term)
- experimental values extracted fitting D_{obs}
- EMPIRE-specific systematics built in
- 'local systematics' created during calculations
- BCS below U_{crt}
- adjustment to discrete levels

Gamma-ray emission

E1, E2, and M1 transitions

- E1 transmission coefficient

$$T_{Xl}^{GMR} = 2\pi f_{Xl}(E_\gamma) E_\gamma^{2l+1} \, .$$

- Brink-Axel hypothesis with
- The E1 γ-ray strength function (Uhl-Kopecky).

$$f_{E1}(E_\gamma) = \sum_{i=1}^{2} \sigma_i \Gamma_i \left[\frac{E_\gamma \Gamma_i(E_\gamma, T)}{(E_\gamma^2 - E_i^2)^2 + E_\gamma^2 \Gamma_i(E_\gamma)^2} + \frac{0.7 \Gamma_i 4\pi^2 T^2}{E^5} \right]$$

Gamma-ray emission (cont.)

- Energy and temperature (T) dependent width

$$\Gamma_i(E_\gamma, T) = \Gamma_i \frac{E_\gamma^2 - 4\pi T^2}{E_i^2} \, .$$

- GDR parameters estimated from the spin dependent systematics.

MSC and MSD coupling

- Higher MSC classes populated directly from the MSD chain
- Incoming flux splits between the first MSD and MSC classes in proportion to the respective state densities and to the average value of the squared matrix elements

$< V_{uu}^2 >$ unbound $\Rightarrow$ unbound
$< V_{ub}^2 >$ unbound $\Rightarrow$ bound

MSC and MSD coupling (cont.)

$$T_1 = T_{om} \frac{R}{(R-1) + \frac{\rho_1(E)}{\rho_1^b(E)}}$$

where $R = < V_{ub}^2 > / < V_{uu}^2 >$

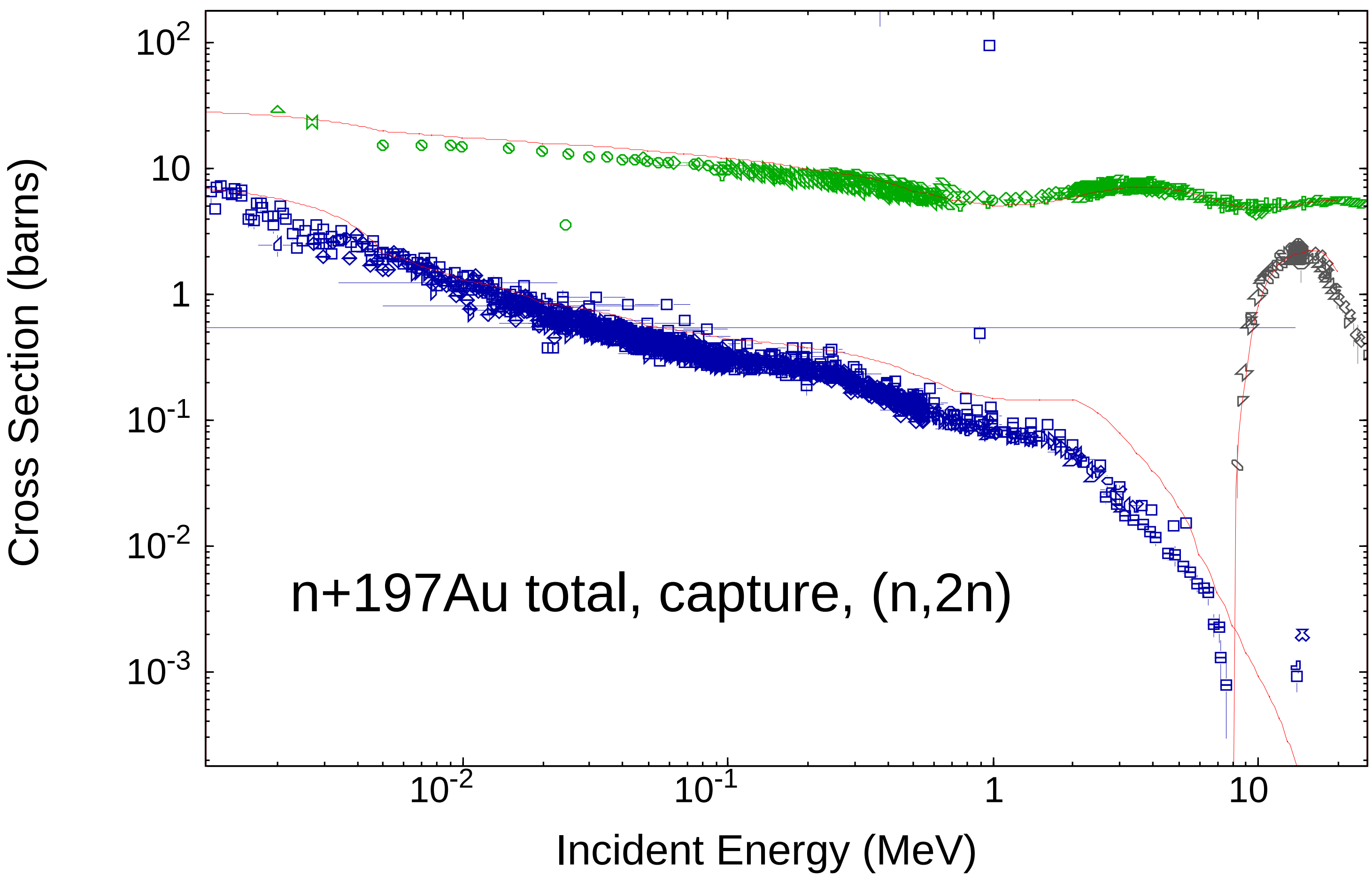
$$T_n = T_{om} - \sum_{i=1}^{n-1} T_i \frac{R}{(R-1) + \frac{\rho_n(E)}{\rho_n^b(E)}}$$

MSC and MSD coupling (cont.)

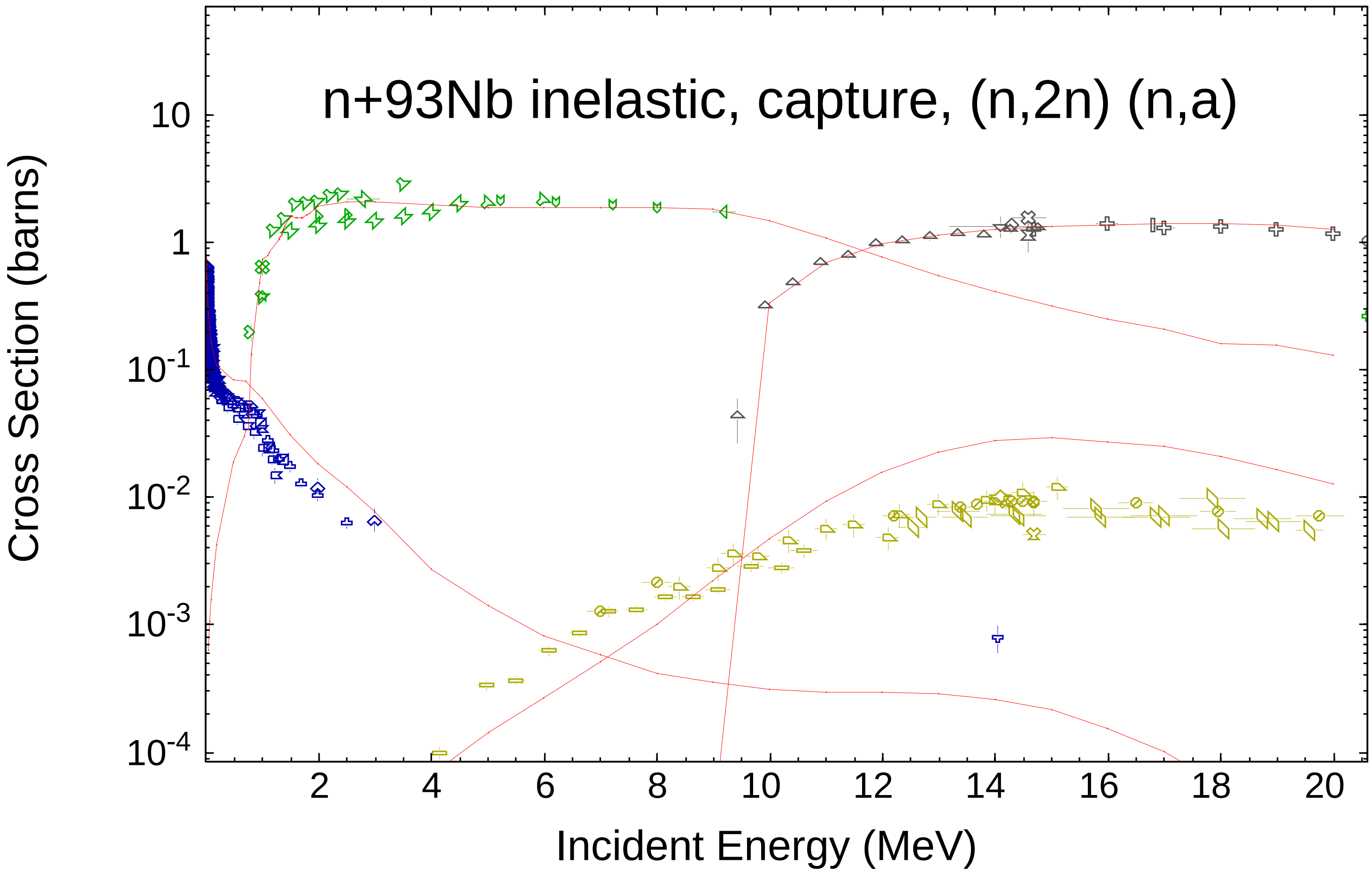
- Absorption cross section available to MSC (σ_{abs}) is reduced by the total MSD emission

$$\sigma_{abs}(J) = \sigma_{OM}(J)\left(1 - \frac{\sigma_{MSD}}{\sigma_{OM}}\right)$$

Default calculations



Default calculations



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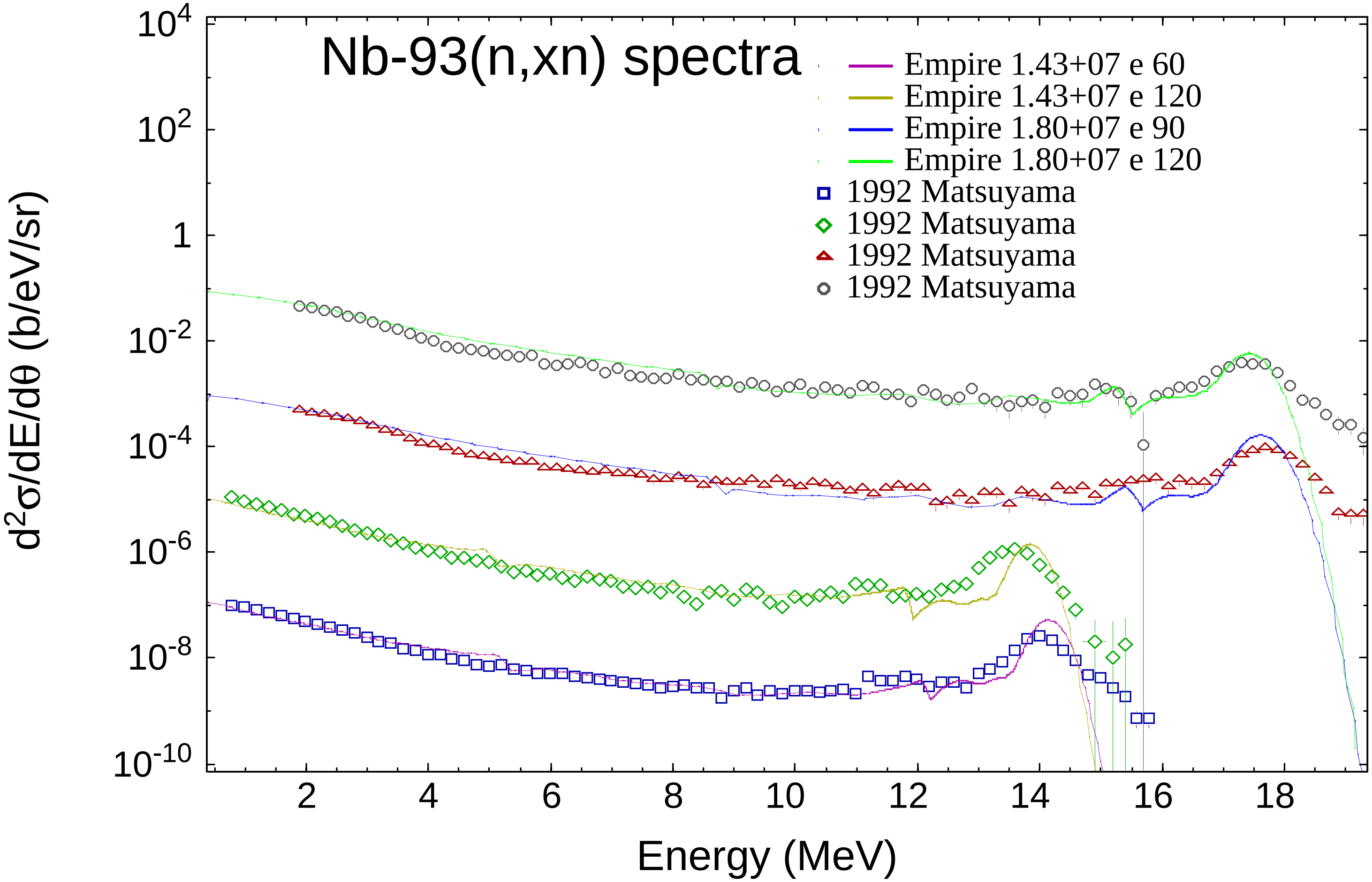

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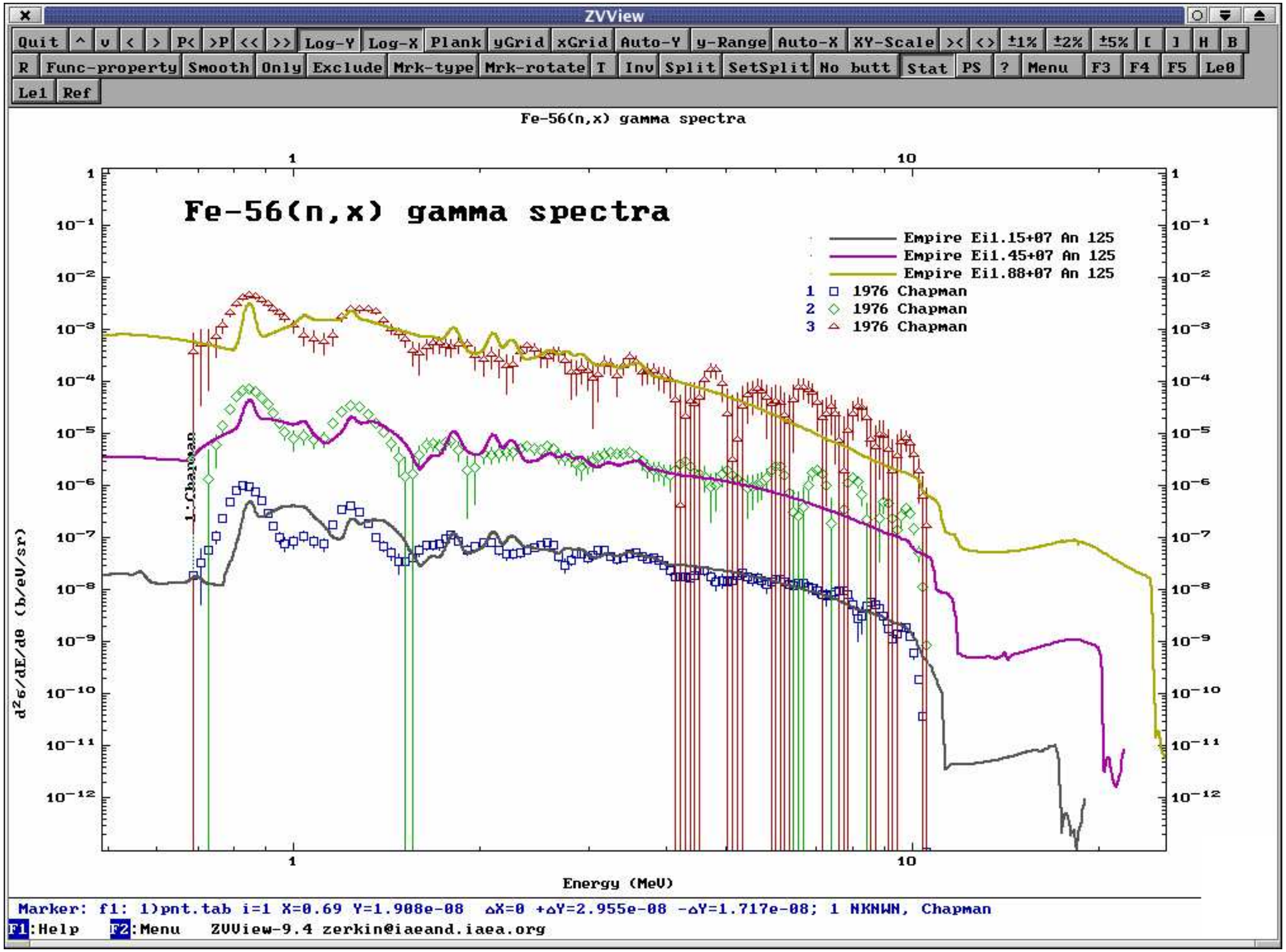
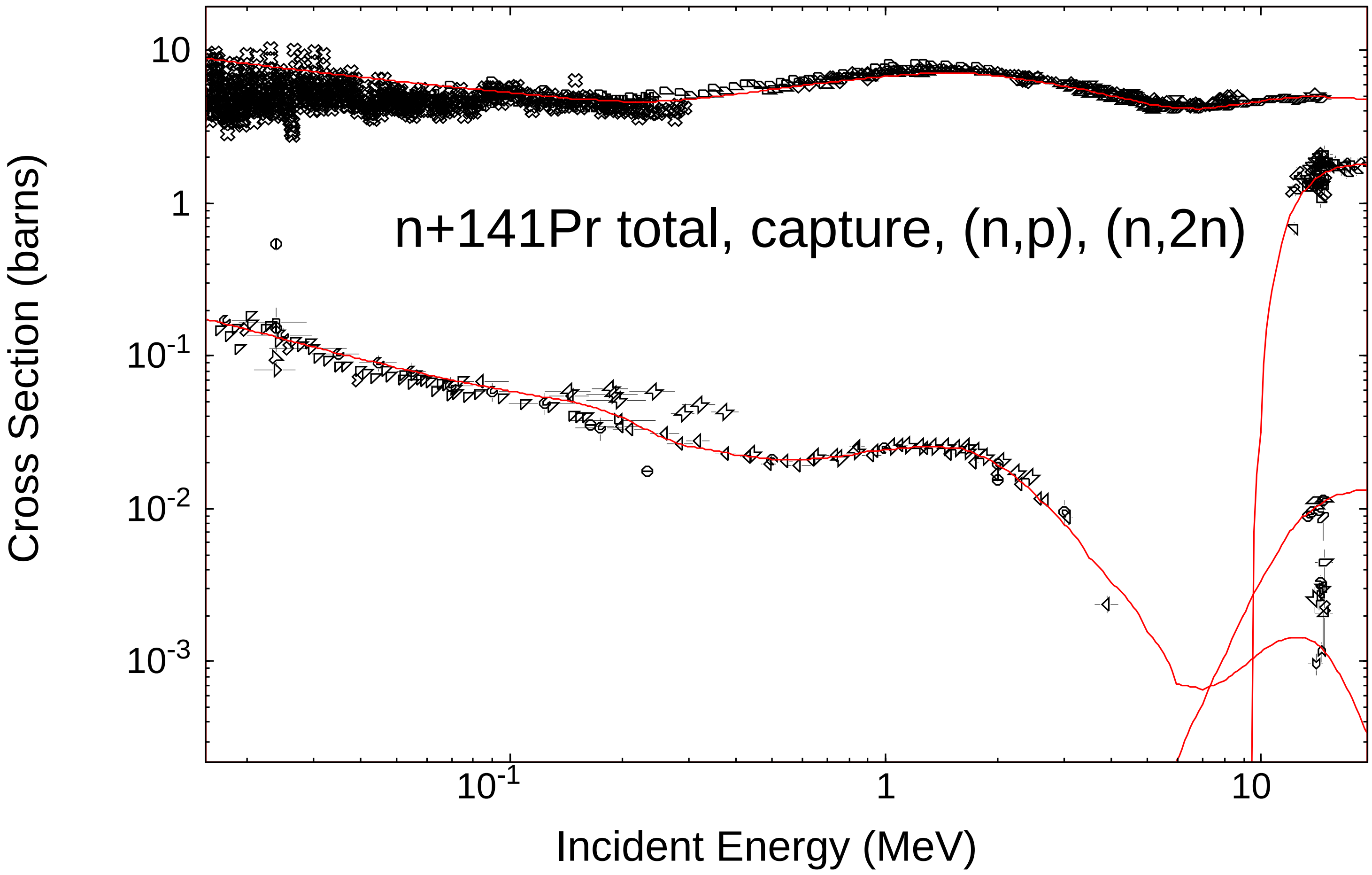
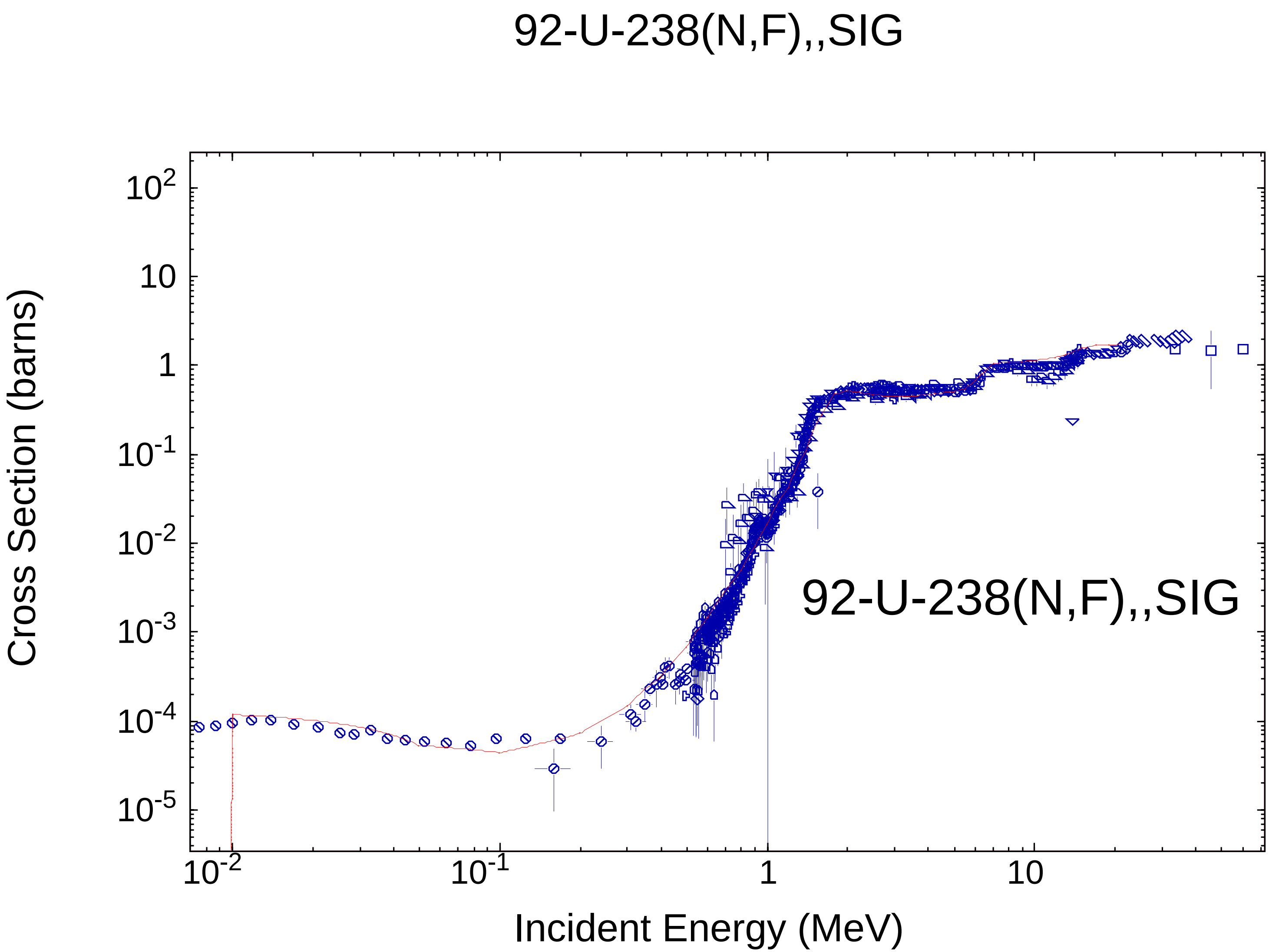


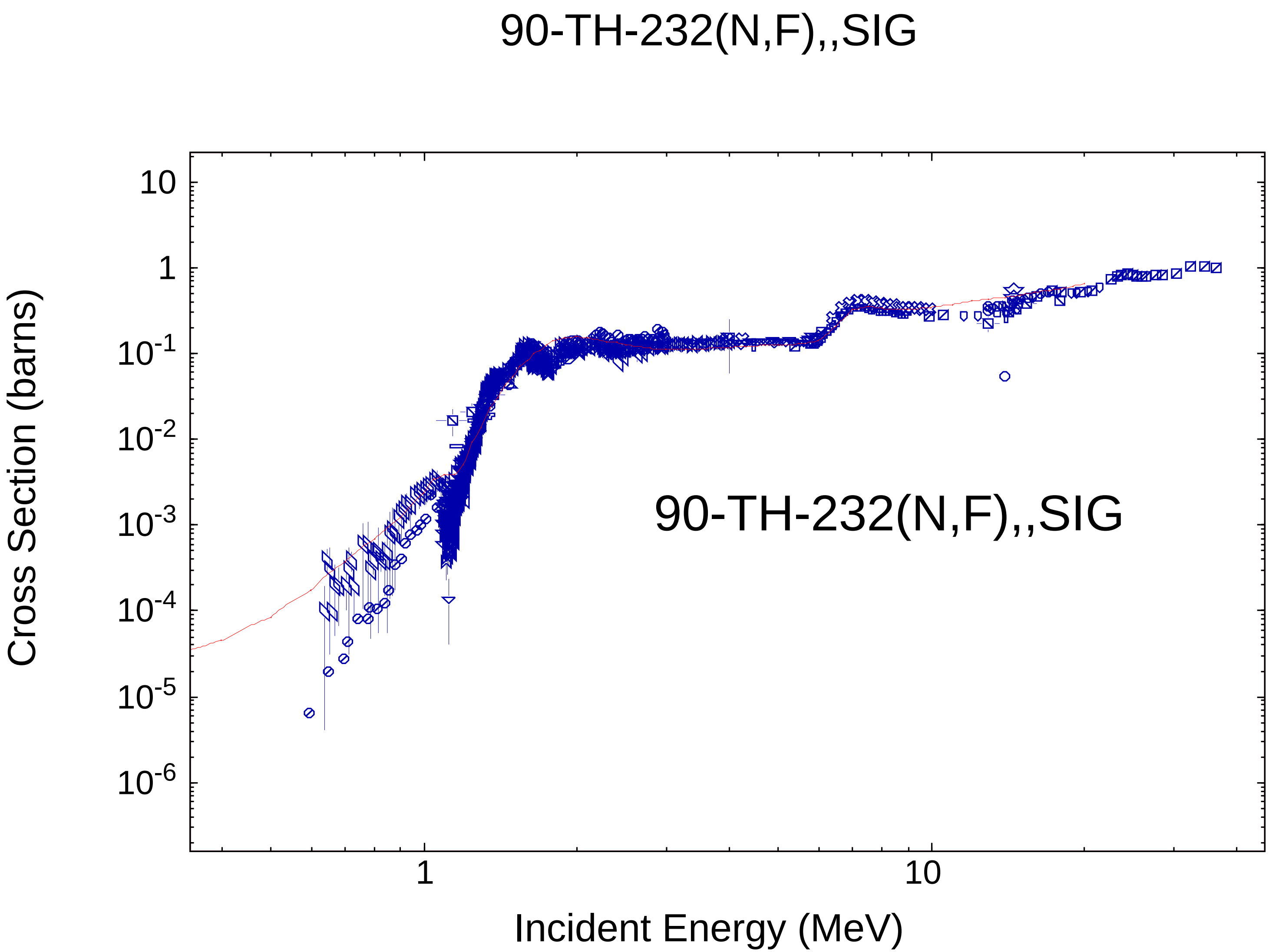
Adjusted calculations (evaluation)



Fission calculations



Fission calculations (cont.)



EMPIRE and surrogate method

Appropriate theoretical tool because of:

- detailed modeling
  - extensive coverage of reaction mechanisms
  - flexible incident channel (including excited targets)
  - observation of spin/parity coupling
  - full gamma cascade
  - good fission model

EMPIRE and surrogate method

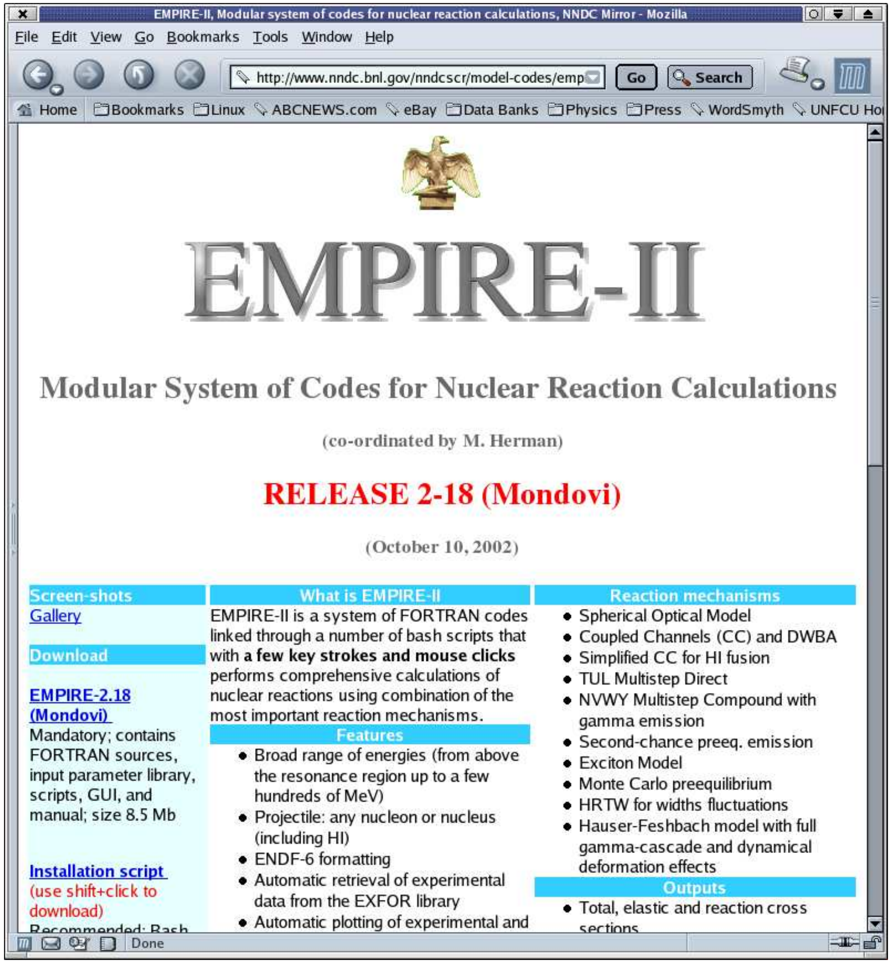
- simultaneous calculations of all major reaction channels (reliability)
- easy to use
  - Graphic User Interface (GUI)
  - simple input (extensive library of default input parameters)
  - automatic comparison with experimental data (adjusting parameters)

How to get EMPIRE

EMPIRE-2.18 (Mondovi) available at:

- http://www.nndc.bnl.gov/nndcscr/model-codes/empire-ii/
- CD-ROM can be requested from: http://www-nds.iaea.org/cd-catalog.html

EMPIRE Web page



Next release of EMPIRE

EMPIRE-2.19 (Lodi) expected March/April 2004 will include:

- new fission channel
- reactions on excited targets
- merging of resonace region into the ENDF file

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